Mirages and enhanced magnetic interactions in quantum corrals

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Abstract. – We develop a theory for the interactions between magnetic impurities in nanoscopic systems. The case of impurities in quantum corrals built on the (111) Cu surface is analyzed in detail. For elliptical corrals with one impurity, clear magnetic mirages are obtained. This leads to an enhancement of the inter-impurity interactions when two impurities are placed at special points in the corral. We discuss the enhancement of the conduction electron response to the local perturbation in other nanoscopic systems.

During the last decade, the physics of nanoscopic and mesoscopic systems has generated an increasing interest in the community due to technological advances that allow for controlled experiments and the possible developments of new applications, nanoelectronics being one example [1].

Coulomb blockade in small metallic or superconducting islands and in quantum dots, the similarities between the physics of quantum dots and Kondo impurities [2] or the observation of spectroscopic mirages in quantum corrals with Kondo impurities [3] make evident that in many aspects interactions and correlations play a central role in the behavior of these small systems. There are some ingredients that distinguish the physics of nanoscopic systems from that of macroscopic samples. One of them, and the most important in the context of the present work, is the quantification of one electron levels due to confinement effects. Here we discuss the interaction between magnetic impurities mediated by conduction electrons, known as the RKKY interaction [4]. We analyze this mechanism in nanoscopic systems and show that in quantum corrals there is a huge enhancement of the impurity-impurity interaction due to confinement effects.

Quantum corrals are built by positioning atoms, typically transition metal atoms, along a closed line on the clean surfaces of noble metals. In recent experiments Manoharan et. al. [3] have built elliptical corrals with Co atoms on the (111) surface of Cu. The Cu (111) surface has a band of surface states, orthogonal to the bulk states, which can be represented as a two dimensional electron gas confined at the surface. The Fermi level is placed at 450 meV above the bottom of the surface state band. The atoms forming the corral act

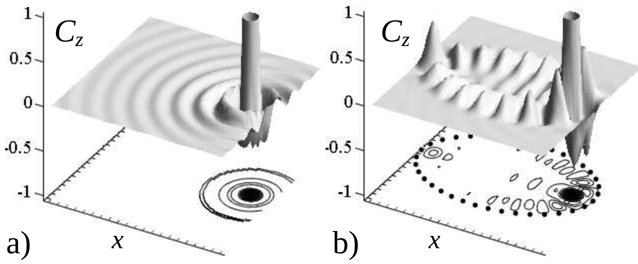

Fig. 1 – Spin correlation functions C_z between the impurity and conduction electron spins (arbitrary units): a) open surface; b) elliptical quantum corral with the impurity at the right focus.

as scattering centers which tend to confine surface electrons inside the corral. If the corral fence where an impenetrable wall electrons inside the corral would be perfectly confined and the energy spectrum would consist of a set of delta functions at the energies of the bound states. The characteristic energy separation between these states decreases as the size of the corral increases. In real systems, there is some *leaking* of the wave function: electrons can tunnel through the fence and the bound states acquire a finite life time. The energy spectrum inside the corral (the local density of states) then consists of resonances, the width of which increases with increasing energy. This structure can drastically change the response of the conduction electrons to a local perturbation. Experiments with different transition metal ipurities inside corrals can be made. Among them, only Co impurities clearly show spectroscopic evidence of Kondo effect. Here we analyze the case of Fe or Ni impurities and describe them with an *s-d* Hamiltonian. We show that the magnetic response is much more pronounced when the impurities are inside the corral rather than on an open surface and in some cases a magnetic mirage is observed. To illustrate these effects we anticipate the results in fig. 1 with the response of the two-dimensional (2D) surface band to a magnetic impurity. When the impurity, interacting via an exchange coupling with the surface electrons, is at a free surface (fig. (1a)), the usual RKKY oscillations in the correlations between the impurity and conduction electron spins are observed. For the 2D case these oscillations decay as the inverse square of the distance to the impurity. When the impurity is placed at the focus of an elliptical corral with a principal axis of $180\mathring{A}$ and eccentricity $\epsilon = 0.75$, the polarization of the surface states is much larger than for the previous case (fig. (1b), note that the scale in figures (1a) and (1b) is the same). Moreover, close to the empty focus of the elliptical corral there is a substantial maximum which could be interpreted as the magnetic mirage of the impurity. These results indicate than under some circumstances two magnetic impurities located at special points of the corral could strongly interact despite of the fact that they could be up to $100\mathring{A}$ apart. The effect is so strong that the impurity-impurity interaction at these large distances could be even larger that the interaction of two impurities placed at short distances on an open surface.

These results where obtained by considering the following Hamiltonian:

$$H = H_{corral} + H_{imp} \tag{1}$$

where H_{corral} describes the surface electrons in the presence of the corral and is given by

$$H_{corral} = \sum_{\sigma} \int d\mathbf{r} \psi_{\sigma}^{\dagger}(\mathbf{r})(-\frac{\hbar^2}{2m^*}\nabla^2 + V_{corral}(\mathbf{r}))\psi_{\sigma}(\mathbf{r}) \tag{2}$$

here $\psi_{\sigma}^{\dagger}(\mathbf{r})$ creates a conduction electron with spin σ at coordinate $\mathbf{r}$, $m^* = 0.3m_e$ is the effective mass of the surface electrons and $V_{corral}(\mathbf{r}) = \sum_i V(\mathbf{r}-\mathbf{R}_i)$ is the potential generated by the atoms forming the corral that are placed at coordinates $\mathbf{R}_i$. We consider typically 36 atoms in the corral fence as in the experiments of reference (3). The second term in Hamiltonian (1) represents a magnetic impurity at coordinate $\mathbf{R}_{imp}$ that interacts with the conduction electron via an exchange interaction J, and in usual notation it reads:

$$H_{imp} = -J\mathbf{S}_{imp} \cdot \psi^{\dagger}(\mathbf{R}_{imp})\hat{\sigma}\psi(\mathbf{R}_{imp}) \tag{3}$$

the operator $\mathbf{S}_{imp}$ describes the impurity spin, the components of $\hat{\sigma}$ are the Pauli matrices and $\psi^{\dagger}(\mathbf{r}) = (\psi_{\uparrow}^{\dagger}(\mathbf{r}), \psi_{\downarrow}^{\dagger}(\mathbf{r}))$. For the *sd*-model considered here, the exchange coupling constant J is positive ($J \simeq 1meV$).

We study diferent geometries: elliptical corrals with eccentricities $\epsilon = 0$, 0.5 and 0.75, and a square corral. To do so, we first calculate the surface-electron propagator in the presence of the corral $G_{\sigma}^{0}(\mathbf{r}, \mathbf{r}', \omega)$ that can be expressed in terms of the free-electron propagator $g_{\sigma}(\mathbf{r}, \mathbf{r}', \omega)$ which in 2D is well known [5]; in the evaluation of this quantity we have used a high energy cutoff. The results inside the ellipse are not very sensitive to the shape of the scattering potential $V(\mathbf{r})$ but to the size and shape of the corral, that is to the coordinates $\mathbf{R}_i$ of the scattering centers. The results presented in this work were obtained with $V(\mathbf{r}) = \alpha\delta(\mathbf{r})$ where $\delta(\mathbf{r})$ is the Dirac delta function. The electron propagator is given by [6]:

$$G_{\sigma}^{0}(\mathbf{r}, \mathbf{r}', \omega) = g_{\sigma}(\mathbf{r}, \mathbf{r}', \omega) + \alpha \sum_{ij} g_{\sigma}(\mathbf{r}, \mathbf{R}_i, \omega)[\mathbf{1} - \alpha\mathbf{g}]_{ij}^{-1} g_{\sigma}(\mathbf{R}_j, \mathbf{r}', \omega) \tag{4}$$

here the matrix $\mathbf{g}$ is defined as $\mathbf{g}_{ij} = g_{\sigma}(\mathbf{R}_i, \mathbf{R}_j, \omega)$.

The total density of states defined as

$$\rho^0(\omega) = -\frac{1}{\pi} \sum_{\sigma} \int_{corral} d\mathbf{r} \, \mathrm{Im}\, G_{\sigma}^{0}(\mathbf{r}, \mathbf{r}, \omega + i0^+) \tag{5}$$

is shown in fig.(2a) and compared with the eigenstates of an isolated ellipse with the same shape and dimensions [7]. For low energies the resonances obtained for the corral are narrow and coincide with the eigenvalues of the isolated system. As the energy increases the resonances become broader and are shifted. This is because for higher energies the fence becomes more transparent, when the electron wave length λ is smaller than the distance d between scattering centers, electrons can easily tunnel through the fence. Figure (2a) also shows the density of states for a corral of the same dimensions made with 24 scattering centers, that has much broader resonances and at the Fermi energy the structure is almost completely washed out. For the elliptical corral used in the rest of the paper with $\epsilon = 0.75$, which reproduces one of the experimental setups of Ref. (3), the Fermi level lies at one well defined resonance. As we discuss below, this coincidence is important and determines the behavior of the system. Finally, the local density of states at the Fermi energy $\rho^0(\mathbf{r}, \varepsilon_F) = -\frac{1}{\pi}\sum_{\sigma} \mathrm{Im}\, G_{\sigma}^{0}(\mathbf{r}, \mathbf{r}, \omega + i0^+)|_{\omega=\varepsilon_F}$ is shown in figs. (2b) and (2c).

Now we consider the case of a magnetic impurity inside the corral and analyze the correlation between the impurity and conduction electron spins. The canonical RKKY calculation is perturbative in the exchange interaction J. In the present case there is no singular scattering as in the Kondo model ($J < 0$) and perturbation theory gives the correct result. An

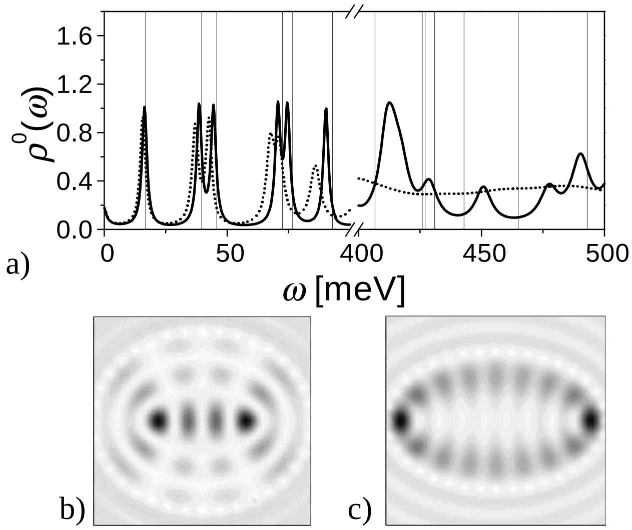

Fig. 2 – a) Total density of states for the elliptical corral with $\epsilon = 0.5$ bounded by 36 (full line) and 24 atoms (dotted line). The vertical lines correspond to the energies of a hard wall corral. b) and c): top view of the local densities of states at the Fermi energy (450 meV) for elliptical corrals with 36 atoms and $\epsilon = 0.5$ and 0.75 respectively

alternative way of doing the calculation is to solve exactly a simpler interaction of the Ising form $S^z_{imp}\psi^\dagger(\mathbf{R}_{imp})\sigma^z\psi(\mathbf{R}_{imp})$. We have shown that in small systems the spin-spin correlations along the z-direction evaluated with the Ising interaction reproduce quantitatively the exact correlations calculated with the full isotropic interaction [8]. For the Ising-type interaction, the electron propagator $G_\sigma(\mathbf{r}, \mathbf{r}', \omega)$ in the presence of the impurity can be evaluated by including and extra spin-dependent scattering center in the matrix $\mathbf{g}$ of Eq. (4) or can be written in terms of $G^0_\sigma(\mathbf{r}, \mathbf{r}', \omega)$ as:

$$G_\sigma(\mathbf{r}, \mathbf{r}', \omega) = G^0_\sigma(\mathbf{r}, \mathbf{r}', \omega) + G^0_\sigma(\mathbf{r}, \mathbf{R}_{imp}, \omega)\Sigma_{imp}(\omega)G^0_\sigma(\mathbf{R}_{imp}, \mathbf{r}', \omega) \tag{6}$$

where

$$\Sigma_{imp}(\omega) = \frac{JS^z_{imp}\sigma}{1 - JS^z_{imp}\sigma G^0_\sigma(\mathbf{R}_{imp}, \mathbf{R}_{imp}, \omega)} \tag{7}$$

This expression is more appropriate to interpret the results. The spin-spin correlation defined as $C^z(\mathbf{R}_{imp}, \mathbf{r}) =< S^z_{imp}\psi^\dagger(\mathbf{r})\sigma^z\psi(\mathbf{r}) >$ can be put into the form

$$C^z(\mathbf{R}_{imp}, \mathbf{r}) = S^z_{imp}\int_{-\infty}^{\varepsilon_F} d\omega[\rho_\uparrow(\mathbf{r}, \omega) - \rho_\downarrow(\mathbf{r}, \omega)] \tag{8}$$

where the spin dependent local densities of states are $\rho_\sigma(\mathbf{r}, \omega) = -\frac{1}{\pi}\,\mathrm{Im}\, G_\sigma(\mathbf{r}, \mathbf{r}, \omega + i0^+)$. If a second impurity is placed at coordinate $\mathbf{R}'_{imp}$ the effective impurity-impurity coupling is proportional to $C^z(\mathbf{R}_{imp}, \mathbf{R}'_{imp})$.

Figures 1 and 3 illustrate the behavior of the correlation function. In Fig. (3a) a cut of $C^z(\mathbf{R}_{imp}, \mathbf{r})$ along the principal axis of the elliptical corral with the impurity at one focus is shown and compared with the same quantity in the absence of the corral, in fig (3b) the

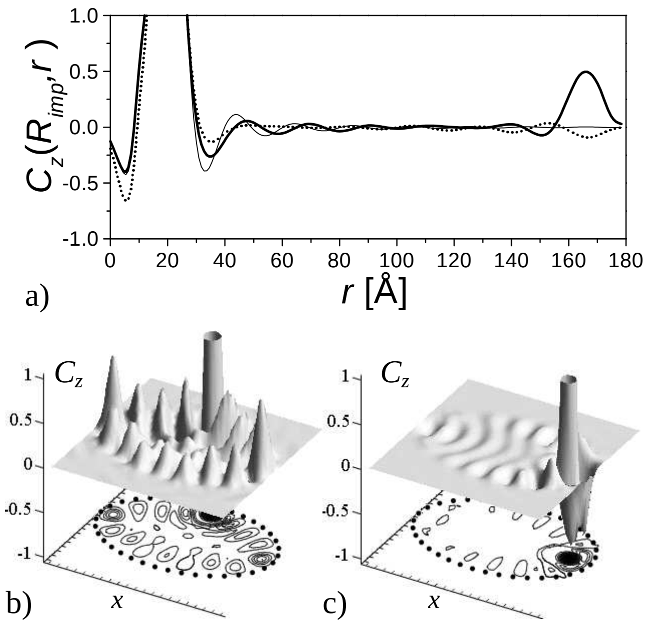

Fig. 3 – a) Spin correlation function C_z along the principal axis with the impurity at the left focus for the *at resonance* (thick line) and *off resonance* (dotted line) situations as compared to the open surface correlations (thin line). b) *At resonance* C_z with the impurity far from the foci; c) *off resonance* C_z with the impurity at the focus

correlation function for the impurity away from the foci is presented. In this last situation again, two well pronounced maxima close to the foci are obtained. At very short distances $C^z(\mathbf{R}_{imp}, \mathbf{r})$ depends on the high energy cutoff, however as $|\mathbf{R}_{imp} - \mathbf{r}|$ increases it rapidly converges to a stable value.

Comparing the results of $C^z(\mathbf{R}_{imp}, \mathbf{r})$ with the local density of states at the Fermi energy (fig (2c)), it is clear that the correlation function reproduces the structure of the unperturbed density of states $\rho^0(\mathbf{r}, \varepsilon_F)$. To understand this rather intuitive result, we consider a simple limit in which both, the coupling constant J and the resonance widths γ inside the corral are small compared to the energy separation $\Delta\varepsilon$ between resonances. Note that for all states around a resonance, the wave function inside the corral is essentially of the same form, differing only outside the corral. To lowest order, the impurity shifts the position of the resonances by $\eta_{\nu,\sigma} \simeq JS^z_{imp}\sigma|\varphi_\nu(\mathbf{R}_{imp})|^2$. Inserting this result into Eqs. (6) and (8), after some algebra and assuming that the Fermi energy coincides with one of the resonant states (*at resonance* situation) we simply obtain $C^z(\mathbf{R}_{imp}, \mathbf{r}) = A|\varphi_{\nu_F}(\mathbf{r})|^2$ where A is a proportionality constant. If the Fermi energy lies between two resonant states (*off resonance* situation), to lowest order the spin-spin correlation is zero. The high response of the conduction electrons obtained for $r \to R_{imp}$ is due to higher order corrections. The occurrence of magnetic mirages of impurities depends on whether the Fermi energy lies at, or close to, one resonance or between two of them, an effect also observed in spectroscopic mirages of Kondo impurities [3]. In quantum corrals, since the Fermi energy is fixed by the bulk material and the position of the resonances depends on the corral size, the system can be designed to have the Fermi level in any of the

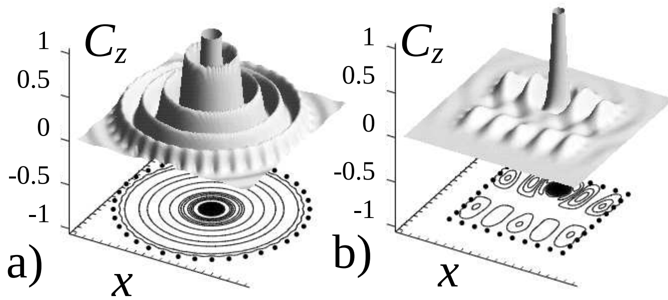

Fig. 4 – Spin correlations C_z for a circular corral with the impurity at the center (a) and for a square corral (b).

two situations. To show the behavior of the conduction electrons response when the Fermi energy is off resonance, instead of changing the corral size, we have shifted the Fermi energy to 428 meV which corresponds to a valley between two resonances in the local density of states. In this case the spin-spin correlation $C^z(\mathbf{R}_{imp}, \mathbf{r})$ shown in figs. (3a) and (3c) presents small amplitude oscillations and an antiferromagnetic correlation with the conduction electrons at the empty focus [8].

As in the case of the spectroscopic mirage of Kondo impurities [9–11], the magnetic mirage obtained in elliptical corrals is due to a symmetry of the system that generates a local density of states at the Fermi level with two pronounced maxima close to the foci. This structure enhances the impurity-impurity interaction if the impurities are placed precisely at, or close to, these points. In all nanoscopic systems however, the local density of states at ε_F shows some structure that will tend to reinforce the magnetic interactions between impurities even if the system geometry is not so special provided that the amplitude $|\varphi_\nu(\mathbf{R}_{imp})|^2$ of the states close to the Fermi level is not too small. In figs. (4a) and (4b) we present the conduction electron response for circular and square corrals. A comparison of these results with that of the impurity at an open surface (fig (1a)), clearly shows the enhancement of the amplitude of the oscillations in the spin- spin correlation due to confinement effects. Similar effects are expected in small metallic grains. During the last decades a lot of work has been done in small metallic clusters with sizes varying from that of a few atoms to macroscopic grains. Magnetic impurities in these systems should behave as in the examples presented above.

Recent advances in STM techniques that allow for the injection of spin-polarized electrons [12] could be used for a direct measurement of the effect in quantum corrals. The spin-polarized current is obtained by using ferromagnetic Fe or Co tips. A small magnetic field $\mathbf{B}$ at low temperatures could be used to orient the impurity spin parallel or antiparallel to the tip magnetization and the difference in the current could be measured at each point. If the impurity spin is parallel to the magnetization tip, the total current is proportional to $a\rho_\uparrow(\mathbf{r}, \varepsilon_F) + b\rho_\downarrow(\mathbf{r}, \varepsilon_F)$ where a and b are characteristic of the tip and are proportional to its majority and minority spin densities of states. For the reverse orientation of the impurity spin the current is $b\rho_\uparrow(\mathbf{r}, \varepsilon_F) + a\rho_\downarrow(\mathbf{r}, \varepsilon_F)$ and the difference is $\Delta j \propto (a-b)[\rho_\uparrow(\mathbf{r}, \varepsilon_F) - \rho_\downarrow(\mathbf{r}, \varepsilon_F)]$. Although the last bracket is not the spin-spin correlation it has the same structure. In fig. 5 the function $\Delta\rho = [\rho_\uparrow(\mathbf{r}, \varepsilon_F) - \rho_\downarrow(\mathbf{r}, \varepsilon_F)]$ is shown for two different cases.

In summary, we have studied the response of conduction electrons with quasi-confined (resonant) states to a local perturbation produced by a magnetic impurity. We have analyzed, using realistic parameters, the case of impurities in quantum corrals. The main conclusions

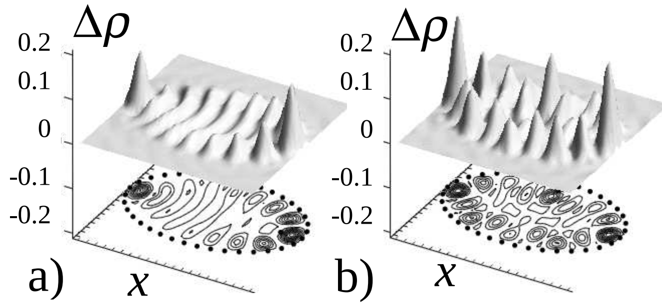

Fig. 5 – $\Delta\rho$ for the impurity at the focus (a) and far from it (b), for the *at resonance* situation

are:

i) If the Fermi energy is at resonance, or close to a resonant state, the response of the conduction electrons to the impurity is strongly enhanced.

ii) If the exchange interaction is small, compared with the typical energy difference of resonances, away from the impurity position the spin-spin correlation function reproduces the structure of the local density of states at the Fermi energy.

iii) Depending on the particular structure of the system, the effective interaction between two impurities could be larger at large distances than at short or intermediate distances. This occurs in elliptical corrals where a magnetic mirage is formed due to the particular structure of the local density of states at the Fermi energy.

iv) A direct measurement of the electron response to the impurity could be made by injecting spin polarized electrons with a ferromagnetic STM tip.

v) Similar effects, produced essentially by the confinement of conduction electrons, are expected in other systems like small metallic clusters or short carbon nanotubes.

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